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Semiclassical theory for transport properties of hard sphere fluid

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Abstract : The statistical mechanical theory is developed to estimate the quantum corrections to the transport properties (TP's) of the semiclassical hard sphere (SCHS) fluid in terms of a classical hard sphere (CHS) fluid of properly chosen hard sphere diameter. The explicit expressions for the shear viscosity and thermal conductivity of the SCHS are given. The numerical results are discussed. The theory is further applied to Ne, where the agreement with the experiment is good at low temperature.

Keywords : Transport properties, shear viscosity, thermal conductivity, semiclassical fluid

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1. Introduction

The transport properties (TP's) of hard sphere fluid aroused considerable interest in recent years [1,2]. Considerable progress has been made in recent years in understanding the TP's of the classical hard sphere fluid [1,2]. However, our understanding of quantum fluids of hard spheres is less satisfactory [3].

In this paper we investigate the quantum corrections to the TP's such as the shear viscosity and thermal conductivity of dense fluid of hard spheres in the semiclassical limit *i.e.* at high temperature. The exchange effect is not considered in the present paper.

2. Basic theory

We consider the semiclassical fluid of hard sphere molecules of diameter σ. The quantum effects modify the hard sphere diameter [4]. However, the structure of a dense semiclassical hard sphere (SCHS) fluid is very similar to that of the classical hard sphere (CHS) fluid of

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the properly choosen hard sphere diameter d. The TP's of the SCHS fluid may be evaluated through the TP's of the CHS fluid.

3. Effective hard sphere diameter

The second virial coefficient B and equation of state $\beta p/\rho$ of the SCHS fluid, correct to the first order quantum correction, are given by [5]

$$B = (2\pi\sigma^3/3)[1+(3/2\sqrt{2})(\lambda/\sigma)] \tag{1}$$

and

$$\beta P/\rho = \{(1+\eta+\eta^2-\eta^3)/(1-\eta)^3\} + 3\sqrt{2}(\lambda/\sigma)\{\eta(1+\eta-(1/2)\eta^2)/(1-\eta)^4\} \tag{2}$$

where λ is the thermal wave length and $\eta = \pi\rho\sigma^3/6$ is the packing fraction.

In order to determine the effective diameter d of the equivalent CHS molecule, we consider the second virial coefficient and equation of state of the CHS fluid. They are given by

$$B = 2\pi d^3/3 \tag{3}$$

and

$$\beta P/\rho = 1+4\eta_d g(d) \tag{4}$$

where $g(d)$ is the radial distribution function (RDF) of the CHS fluid at the contact and $\eta_d = \pi\rho d^3/6 = \eta d^{\wedge 3}$ where $d^\wedge = d/\sigma$.

Equating eqs. (1) and (3), the effective hard sphere diameter (EHSD) d is expressed by

$$d^\wedge = \left[1+(3/2\sqrt{2})(\lambda/\sigma)\right]^{1/3} \approx 1+(1/2\sqrt{2})(\lambda/\sigma) \tag{5}$$

Thus the quantum effects for the hard sphere fluid is taken into account by replacing the actual diameter σ by an effective diameter $\sigma[1+(1/2\sqrt{2})(\lambda/\sigma)]$. This is in accordance with the result found previously [4].

Similarly equating eqs. (2) and (4), the RDF $g(d)$ of the CHS fluid is given by

$$g(d) = g^c(\sigma)\left[1+(3/2\sqrt{2})\alpha(\lambda/\sigma)\right]\left[1+(3/2\sqrt{2})(\lambda/\sigma\right]^{-1} \tag{6}$$

where $g^c(\sigma)$ is the RDF of the CHS fluid of the diameter σ at the contact and given by [6].

$$g^c(\sigma) = (1-\eta/2)(1-\eta)^{-3}, \tag{7}$$

and α is the correction coefficient

$$\alpha = (1+\eta-\eta^2/2)/(1-\eta/2)^{-1}(1-\eta)^{-1} \tag{8}$$

4. Transport properties of semiclassical hard sphere fluid

We employ the revised Enskog theory (RET) of Beijener and Ernst [1] to estimate the shear viscosity μ and thermal conductivity K of the CHS fluid. They are given by [1]

$$\mu = g(d)^{-1}\left[1+(4/5)(4\eta_d g(d))+0.7615(4\eta_d g(d))^2\right]\mu_0 \tag{9}$$

$$K = g(d)^{-1}\left[1 + (6/5)(4\eta_d g(d)) + 0.7575(4\eta_d g(d))^2\right]K_0 \tag{10}$$

where
$$\mu_0 = (5/16\pi d^2)(2\pi mkT)^{1/2} = \mu_0^c / d^{\wedge 2} \tag{11}$$

$$K_0 = (75k/64\pi d^2)(\pi kT/m)^{1/2} = K_0^c / d^{\wedge 2} \tag{12}$$

with
$$\mu_0^c = (5/16\pi\sigma^2)(2\pi mkT)^{1/2} \tag{13}$$

$$K_0^c = (75k/64\pi\sigma^2)(\pi kT/m)^{1/2} \tag{14}$$

Here μ_0^c and K_0^c are, respectively, the shear viscosity and thermal conductivity of the ideal classical gas. m is the mass of a molecule and T is the absolute temperature.

With the help of eqs. (5) and (6), eq. (9) can be expressed as

$$\mu^* \equiv \mu/\mu_0^c = \left[\mu_c^* + (1/2\sqrt{2})\mu_1^*(\lambda/\sigma)\right]\left[1 + (3/2\sqrt{2})\alpha(\lambda/\sigma)\right]^{-1} \tag{15}$$

where
$$\mu_c^* \equiv \mu_c/\mu_0^c = g^c(\sigma)^{-1}\left[1 + (4/5)(4\eta g^c(\sigma)) + 0.7615(4\eta g^c(\sigma))^2\right] \tag{16}$$

is the shear viscosity of the CHS fluid and

$$\mu_1^* \equiv \mu_c^* + 3\alpha g^c(\sigma)^{-1}\left[(4/5)(4\eta g^c(\sigma)) + 1.5230(4\eta g^c(\sigma))^2\right] \tag{17}$$

is the first order quantum correction coefficient to it.

Similarly from eq. (10), we obtain an expression for K

$$K^* \equiv K/K_0^c = \left[K_c^* + (1/2\sqrt{2})K_1^*(\lambda/\sigma)\right]\left[1 + (3/2\sqrt{2})\alpha(\lambda/\sigma)\right]^{-1} \tag{18}$$

where
$$K_c^* = g^c(\sigma)^{-1}\left[1 + (6/5)(4\eta g^c(\sigma)) + 0.7575(4\eta g^c(\sigma))^2\right] \tag{19}$$

is the thermal conductivity of the CHS fluid and

$$K_1^* = K_c^* + 3\alpha g^c(\sigma)^{-1}\left[(6/5)(4\eta g^c(\sigma)) + 1.5150(4\eta g^c(\sigma))^2\right] \tag{20}$$

is the first order quantum correction coefficient to it.

We have calculated the shear viscosity μ^* (using eqs. (9) and (15)) and thermal conductivity K^* (using eqs. (10) and (18)) for a range of packing fraction η at $\lambda/\sigma = 0$ and

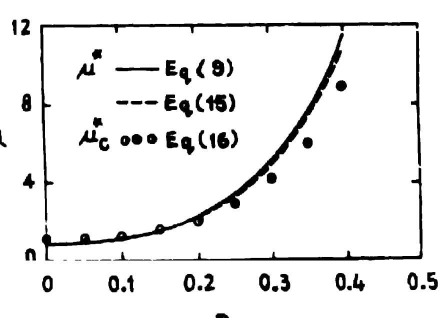

Figure 1. The shear viscosity μ^* of the hard sphere as a function of η at $\lambda/\sigma = 0$ and 0.1.

0.1. $\lambda/\sigma = 0$ corresponds to the classical values. These values are shown in Figures 1 and 2 as a function of η. The values of μ^* and K^* obtained under different approximations are comparable at low η and begin to deviate with increase of η. The quantum effects decrease the values at low value of η ($\eta \leq 0.10$) while increase them for $\eta \geq 0.15$.

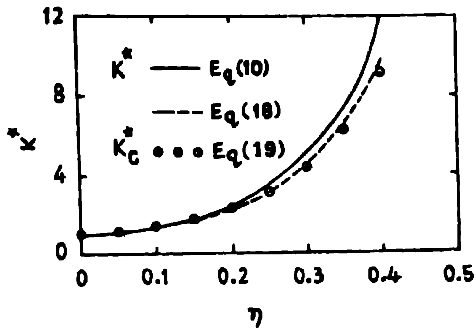

Figure 2. Thermal conductivity K^* of the hard sphere as a function of η at $\lambda/\sigma = 0$ and 0.1.

5. Transport properties of real fluids

This theory can be applied to estimate the TP's of real fluids such as Ne whose molecules interact *via* the Lennard-Jones (12–6) potential. For such a system, $\Lambda^* = h/\sigma^2\sqrt{m/\varepsilon}$ is the quantum parameters.

No experimental results are available for dense semiclassical fluids. In order to test the accuracy of our theory, we apply it to calculate μ and K of dilute Ne gas and compare with the experimental data [3] as well as those obtained previously by us [7]. The agreement with the experiment is good at low temperature and decrease with increase of temperature. On the other hand, the previous results [7] are good at high temperature and deviate with decrease of temperature. Thus these two methods are complimentary to each other.

Table 1. Shear viscosity μ and thermal conductivity λ for Ne.

$\mu \times 10^7$ (g. cm^{-1}sec.$^{-1}$)				$K \times 10^7$ (Cal. cm^{-1} sec.$^{-1}$ deg^{-1})			
$\bar{T}$(k)	Present theory	Previous theory	Expt.	T(k)	Present theory	Previous theory	Expt.
80	1280	1366	1198	90.2	505	562	489
120	1596	1803	1646	273.2	914	1102	1092
160	1968	2108	2026	373.2	1077	1341	1357
200	2099	2425	2376				

6. Summary

The purpose of the present paper is to develop a theory for quantum corrections to the TP's of the SCHS fluid using the EHSD method. This theory is applied to estimate the TP's of Ne. The agreement is good.

Acknowledgment

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